

Electronic Supplementary Information

DFT Studies on Quantum Mechanical Tunneling in Tautomerization of Three-membered Rings

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Table S1: The activation energy barrier as well as the stability of the tautomeric forms calculated at Gaussian G2 method have been given in kcal/mol.

	$\Delta G^\ddagger$	ΔG
1	63.4	-6.8
2	-	-17.3
3	72.7	4.3
4	-	6.3
5	58.3	-10.4
1-W	32.7	-9.1
2-W	35.6	-18.8
3-W	39.1	0.4
4-W	22.1	3.7
5-W	19.4	-11.1

Table S2: QMT rate constants calculated at M062X/6-311+G(d,p) level of theory

		5		5-D		
T	CVT	SCT	κ	CVT	SCT	κ
50	1.41-242	6.27E-46	#VALUE!	1.68-246	8.30E-85	#VALUE!
75	8.54-158	5.72E-41	#VALUE!	2.05-160	8.30E-67	#VALUE!
100	2.32-115	2.44E-38	#VALUE!	2.48-117	9.71E-58	#VALUE!
125	7.07E-90	1.54E-36	2.18E+53	1.85E-91	3.69E-52	1.99E+39
150	7.18E-73	5.18E-35	7.21E+37	3.39E-74	3.56E-48	1.05E+26
175	1.03E-60	1.87E-33	1.82E+27	7.42E-62	7.90E-45	1.06E+17
200	1.39E-51	9.37E-32	6.74E+19	1.36E-52	1.38E-41	1.01E+11
225	1.77E-44	5.79E-30	3.27E+14	2.20E-45	2.50E-38	1.14E+07
250	8.63E-39	3.80E-28	4.40E+10	1.30E-39	4.02E-35	3.09E+04
273	1.79E-34	1.79E-26	1.00E+08	3.11E-35	2.86E-32	9.20E+02
275	3.93E-34	2.50E-26	6.36E+07	6.91E-35	5.01E-32	7.25E+02
298	1.56E-30	1.15E-24	7.37E+05	3.09E-31	2.69E-29	8.71E+01
300	3.02E-30	1.61E-24	5.33E+05	6.03E-31	4.58E-29	7.60E+01
325	5.88E-27	9.67E-23	1.64E+04	1.31E-27	2.74E-26	2.09E+01
350	3.91E-24	5.21E-21	1.33E+03	9.54E-25	9.43E-24	9.88E+00
375	1.09E-21	2.42E-19	2.22E+02	2.90E-22	1.78E-21	6.14E+00
400	1.52E-19	9.54E-18	6.28E+01	4.32E-20	1.92E-19	4.44E+00
425	1.19E-17	3.09E-16	2.60E+01	3.59E-18	1.26E-17	3.51E+00
450	5.72E-16	8.03E-15	1.40E+01	1.83E-16	5.38E-16	2.94E+00
500	4.18E-13	2.70E-12	6.46E+00	1.47E-13	3.35E-13	2.28E+00
1000	3.77E+00	5.20E+00	1.38E+00	2.06E+00	2.40E+00	1.17E+00
1500	8.75E+04	9.75E+04	1.11E+00	5.50E+04	5.70E+04	1.04E+00
2000	1.38E+07	1.43E+07	1.04E+00	9.21E+06	9.15E+06	9.93E-01

		1-W		1-W-D		
T	CVT	SCT	κ	CVT	SCT	κ
50	4.30E-91	1.59E-15	3.70E+75	2.59E-94	6.55E-23	2.53E+71

75	4.91E-57	4.98E-15	1.01E+42	3.39E-59	3.50E-22	1.03E+37
100	4.69E-40	2.09E-14	4.46E+25	1.08E-41	3.64E-21	3.37E+20
125	6.51E-30	1.50E-13	2.30E+16	3.04E-31	1.16E-19	3.82E+11
150	3.47E-23	1.67E-12	4.81E+10	2.57E-24	8.04E-18	3.13E+06
175	2.08E-18	2.42E-11	1.16E+07	2.14E-19	8.18E-16	3.82E+03
200	7.63E-15	3.89E-10	5.10E+04	9.97E-16	1.03E-13	1.03E+02
225	4.37E-12	6.32E-09	1.45E+03	6.86E-13	1.24E-11	1.81E+01
250	6.83E-10	9.97E-08	1.46E+02	1.25E-10	9.58E-10	7.66E+00
273	3.10E-08	1.17E-06	3.77E+01	6.32E-09	3.08E-08	4.87E+00
275	4.19E-08	1.44E-06	3.44E+01	8.61E-09	4.07E-08	4.73E+00
298	9.89E-07	1.46E-05	1.48E+01	2.24E-07	7.86E-07	3.51E+00
300	1.27E-06	1.77E-05	1.39E+01	2.90E-07	9.98E-07	3.44E+00
325	2.26E-05	1.76E-04	7.79E+00	5.61E-06	1.55E-05	2.76E+00
350	2.64E-04	1.38E-03	5.23E+00	7.06E-05	1.65E-04	2.34E+00
375	2.20E-03	8.69E-03	3.95E+00	6.29E-04	1.30E-03	2.07E+00
400	1.40E-02	4.48E-02	3.20E+00	4.25E-03	7.95E-03	1.87E+00
425	7.14E-02	1.94E-01	2.72E+00	2.28E-02	3.94E-02	1.73E+00
450	3.02E-01	7.20E-01	2.38E+00	1.01E-01	1.64E-01	1.62E+00

		2-W		2-W-D		
T	CVT	SCT	κ	CVT	SCT	κ
50	6.94-107	2.69E-17	#VALUE!	8.85-111	1.64E-24	#VALUE!
75	1.57E-67	2.20E-16	1.40E+51	3.90E-70	1.45E-23	3.72E+46
100	6.90E-48	2.73E-15	3.96E+32	7.44E-50	3.45E-22	4.64E+27
125	3.88E-36	3.71E-14	9.56E+21	9.99E-38	1.24E-20	1.24E+17
150	2.48E-28	5.05E-13	2.04E+15	1.13E-29	5.76E-19	5.10E+10
175	8.84E-23	6.49E-12	7.34E+10	5.99E-24	3.32E-17	5.54E+06
200	1.24E-18	7.83E-11	6.31E+07	1.13E-19	2.11E-15	1.87E+04
225	2.04E-15	8.99E-10	4.41E+05	2.32E-16	1.27E-13	5.47E+02
250	7.43E-13	1.01E-08	1.36E+04	1.01E-13	6.54E-12	6.48E+01
273	6.42E-11	8.95E-08	1.39E+03	1.00E-11	2.01E-10	2.01E+01
275	9.12E-11	1.08E-07	1.18E+03	1.44E-11	2.67E-10	1.85E+01
298	3.70E-09	8.85E-07	2.39E+02	6.52E-10	6.05E-09	9.28E+00
300	4.96E-09	1.06E-06	2.14E+02	8.84E-10	7.82E-09	8.85E+00
325	1.45E-07	9.17E-06	6.32E+01	2.86E-08	1.58E-07	5.52E+00
350	2.59E-06	6.90E-05	2.66E+01	5.58E-07	2.24E-06	4.01E+00
375	3.13E-05	4.47E-04	1.43E+01	7.29E-06	2.33E-05	3.20E+00
400	2.76E-04	2.49E-03	9.02E+00	6.89E-05	1.85E-04	2.69E+00
425	1.88E-03	1.20E-02	6.38E+00	4.99E-04	1.17E-03	2.34E+00
450	1.03E-02	5.02E-02	4.87E+00	2.89E-03	6.09E-03	2.11E+00

		3-W		3-W-D		
T	CVT	SCT	κ	CVT	SCT	κ
50	8.55-125	5.86E-27	#VALUE!	3.75-128	4.23E-36	#VALUE!
75	1.53E-79	5.05E-25	3.30E+54	8.67E-82	1.92E-33	2.21E+48
100	5.89E-57	5.99E-23	1.02E+34	1.17E-58	9.41E-31	8.04E+27
125	1.91E-43	5.75E-21	3.01E+22	7.97E-45	4.40E-28	5.52E+16
150	1.80E-34	3.91E-19	2.17E+15	1.22E-35	1.57E-25	1.29E+10

175	4.35E-28	1.84E-17	4.23E+10	4.15E-29	3.66E-23	8.82E+05
200	2.56E-23	6.34E-16	2.48E+07	3.14E-24	7.69E-21	2.45E+03
225	1.27E-19	1.71E-14	1.35E+05	1.89E-20	1.72E-18	9.10E+01
250	1.12E-16	4.04E-13	3.61E+03	1.94E-17	3.48E-16	1.79E+01
273	1.89E-14	6.88E-12	3.64E+02	3.68E-15	3.06E-14	8.32E+00
275	2.84E-14	8.77E-12	3.09E+02	5.57E-15	4.40E-14	7.90E+00
298	2.01E-12	1.36E-10	6.77E+01	4.33E-13	2.20E-12	5.08E+00
300	2.81E-12	1.72E-10	6.12E+01	6.13E-13	3.02E-12	4.93E+00
325	1.36E-10	2.92E-09	2.15E+01	3.24E-11	1.17E-10	3.61E+00
350	3.75E-09	4.06E-08	1.08E+01	9.64E-10	2.80E-09	2.90E+00
375	6.59E-08	4.50E-07	6.83E+00	1.81E-08	4.48E-08	2.48E+00
400	8.06E-07	3.97E-06	4.93E+00	2.36E-07	5.12E-07	2.17E+00
425	7.31E-06	2.82E-05	3.86E+00	2.26E-06	4.43E-06	1.96E+00
450	5.17E-05	1.66E-04	3.21E+00	1.68E-05	3.03E-05	1.80E+00

		4-W		4-W-D		
T	CVT	SCT	κ	CVT	SCT	κ
50	4.74E-62	3.77E-15	7.95E+46	5.26E-66	5.19E-22	9.88E+43
75	1.77E-37	1.49E-12	8.43E+24	4.02E-40	5.96E-19	1.48E+21
100	3.42E-25	2.25E-10	6.59E+14	3.44E-27	3.44E-16	1.00E+11
125	7.77E-18	1.52E-08	1.96E+09	1.91E-19	1.24E-13	6.47E+05
150	6.04E-13	5.79E-07	9.58E+05	2.66E-14	2.55E-11	9.61E+02
175	1.83E-09	1.41E-05	7.71E+03	1.21E-10	4.89E-09	4.03E+01
200	7.29E-07	2.68E-04	3.68E+02	6.56E-08	6.70E-07	1.02E+01
225	7.52E-05	4.34E-03	5.77E+01	8.59E-06	4.44E-05	5.17E+00
250	3.03E-03	5.73E-02	1.89E+01	4.17E-04	1.45E-03	3.49E+00
273	4.94E-02	4.86E-01	9.84E+00	7.85E-03	2.14E-02	2.73E+00
275	6.17E-02	5.78E-01	9.38E+00	9.87E-03	2.66E-02	2.69E+00
298	6.27E-01	3.79E+00	6.04E+00	1.13E-01	2.56E-01	2.27E+00
300	7.54E-01	4.43E+00	5.87E+00	1.37E-01	3.05E-01	2.23E+00
325	6.22E+00	2.63E+01	4.23E+00	1.25E+00	2.46E+00	1.96E+00
350	3.76E+01	1.26E+02	3.34E+00	8.36E+00	1.48E+01	1.77E+00
375	1.78E+02	4.95E+02	2.78E+00	4.30E+01	7.05E+01	1.64E+00
400	6.94E+02	1.68E+03	2.41E+00	1.79E+02	2.75E+02	1.54E+00
425	2.29E+03	4.93E+03	2.16E+00	6.32E+02	9.22E+02	1.46E+00
450	6.62E+03	1.30E+04	1.97E+00	1.93E+03	2.70E+03	1.40E+00

		5-W		5-W-D		
T	CVT	SCT	κ	CVT	SCT	κ
50	6.40E-49	4.17E-04	6.52E+44	3.55E-53	1.90E-09	5.35E+43
75	9.62E-29	1.24E-03	1.29E+25	1.39E-31	6.81E-09	4.90E+22
100	1.16E-18	3.98E-03	3.43E+15	8.45E-21	2.74E-08	3.24E+12
125	1.25E-12	1.38E-02	1.10E+10	2.38E-14	1.73E-07	7.27E+06
150	1.27E-08	5.16E-02	4.06E+06	4.53E-10	2.42E-06	5.34E+03
175	8.99E-06	2.12E-01	2.36E+04	4.97E-07	6.91E-05	1.39E+02
200	1.20E-03	1.03E+00	8.58E+02	9.20E-05	2.20E-03	2.39E+01
225	5.33E-02	5.88E+00	1.10E+02	5.21E-03	4.89E-02	9.39E+00
250	1.09E+00	3.44E+01	3.16E+01	1.29E-01	6.95E-01	5.39E+00

273	1.06E+01	1.60E+02	1.51E+01	1.46E+00	5.58E+00	3.82E+00
275	1.27E+01	1.82E+02	1.43E+01	1.76E+00	6.59E+00	3.74E+00
298	8.38E+01	7.27E+02	8.68E+00	1.31E+01	3.87E+01	2.95E+00
300	9.74E+01	8.15E+02	8.37E+00	1.54E+01	4.47E+01	2.90E+00
325	5.41E+02	3.09E+03	5.71E+00	9.55E+01	2.30E+02	2.41E+00
350	2.34E+03	1.01E+04	4.32E+00	4.54E+02	9.50E+02	2.09E+00
375	8.27E+03	2.86E+04	3.46E+00	1.74E+03	3.27E+03	1.88E+00
400	2.49E+04	7.24E+04	2.91E+00	5.63E+03	9.70E+03	1.72E+00
425	6.54E+04	1.66E+05	2.54E+00	1.58E+04	2.54E+04	1.61E+00
450	1.54E+05	3.49E+05	2.27E+00	3.95E+04	5.99E+04	1.52E+00

Table S3: Rate constants calculated using Eyring-Polanyi at 298.15 K have compared with the CVT rate constants calculated at 298 K.

	Eyring-Polanyi	CVT	
1	2.91E-33	-	
2	9.92E-35	-	
3	3.13E-40	-	
4	8.01E-33	-	
5	1.50E-30	1.56E-30	
1-W	4.01E-06	9.89E-07	
2-W	3.94E-09	3.70E-09	
3-W	1.97E-12	2.01E-12	
4-W	9.06E-01	6.27E-01	
5-W	8.66E+01	8.38E+01	
1-2W	1.70E+02	-	
2-2W	4.90E+00	-	
3-2W	1.75E-03	9.30E-04	
4-2W	1.96E+07	-	
5-2W	1.49E+08	1.35E+08	

Table S4: The activation free energy and reaction energies for 1-5 in the presence of the two water molecule calculated at the M062X/6-311+G(d,p) level of theory are given in kcal/mol.

	$\Delta E_{\text{ZPE}}^{\#}$	ΔE_{ZPE}	$\Delta G^{\#}$	ΔG
1-2W	13.0	-13.4	14.4	-13.7
2-2W	14.8	-21.2	16.5	-22.4
3-2W	19.3	-3.9	21.2	-3.9
4-2W	5.7	-0.3	7.5	0.3
5-2W	4.6	-11.0	6.3	-11.1

Table S5: QMT rate constants calculated at M062X/6-311+G(d,p) level of theory for two water assisted tautomerization process of **3** and **5**.

	3-2W			5-2W		
	CVT	SCT	κ	CVT	SCT	κ
50	2.38E-74	1.23E-19	5.17E+54	2.00E-09	1.02E+05	5.10E+13
75	8.06E-46	8.77E-18	1.09E+28	1.59E-02	2.95E+05	1.86E+07
100	1.39E-31	1.51E-15	1.09E+16	4.29E+01	9.92E+05	2.31E+04

125	4.40E-23	1.93E-13	4.39E+09	4.65E+03	3.49E+06	7.51E+02
150	1.89E-17	1.81E-11	9.58E+05	1.00E+05	1.10E+07	1.10E+02
175	1.86E-13	1.23E-09	6.61E+03	8.64E+05	2.92E+07	3.38E+01
200	1.75E-10	5.79E-08	3.31E+02	4.20E+06	6.55E+07	1.56E+01
225	3.44E-08	1.88E-06	5.47E+01	1.40E+07	1.27E+08	9.07E+00
250	2.28E-06	4.13E-05	1.81E+01	3.60E+07	2.20E+08	6.11E+00
273	5.34E-05	5.05E-04	9.46E+00	7.24E+07	3.36E+08	4.64E+00
275	6.85E-05	6.19E-04	9.04E+00	7.65E+07	3.48E+08	4.55E+00
298	9.30E-04	5.45E-03	5.86E+00	1.35E+08	4.97E+08	3.68E+00
300	1.14E-03	6.50E-03	5.70E+00	1.41E+08	5.12E+08	3.63E+00
325	1.22E-02	5.00E-02	4.10E+00	2.35E+08	7.10E+08	3.02E+00
350	9.14E-02	2.96E-01	3.24E+00	3.60E+08	9.40E+08	2.61E+00
375	5.18E-01	1.40E+00	2.70E+00	5.17E+08	1.20E+09	2.32E+00
400	2.34E+00	5.49E+00	2.35E+00	7.05E+08	1.48E+09	2.10E+00
425	8.82E+00	1.84E+01	2.09E+00	9.22E+08	1.78E+09	1.93E+00
450	2.84E+01	5.41E+01	1.90E+00	1.16E+09	2.10E+09	1.81E+00

M062X/6-311+G(d,p) level of theory optimized Cartesian coordinates

1				1-TS				1-P			
C	-0.00000500	1.22729900	-0.00009600	C	0.03627800	1.12579000	-0.00857800	C	-0.04122300	1.18821500	0.00004700
C	0.74183400	-0.09630500	0.00024000	C	-0.80115000	-0.03535100	0.02584100	C	-0.82635200	-0.00957700	0.00000400
C	-0.74182000	-0.09633600	0.00024800	C	0.62826100	-0.19229800	-0.10221200	C	0.60190200	0.00757100	-0.00036400
O	1.80754300	-0.61540600	-0.00013100	O	-1.90653700	-0.48219300	0.01389700	O	-1.88270100	-0.57159100	0.00007100
H	-0.00002700	1.81924800	0.91621500	H	0.05047300	2.20576600	-0.08866600	H	0.03586100	2.26621700	0.00015600
H	0.00004600	1.81920800	-0.91641700	H	1.38366600	0.71331000	0.36680600	H	2.48468000	0.04006100	0.00054300
O	-1.80755200	-0.61539400	-0.00013800	O	1.82972800	-0.55629600	0.01504800	O	1.76688800	-0.60635000	0.00007600
2				2-TS				2-P			
C	-1.24711600	-0.13974400	0.00000000	C	0.05114000	1.15121500	0.00625700	C	1.22107800	0.00546800	0.00000000
C	0.13045100	-0.74243100	0.00000000	C	0.83688100	-0.01133000	-0.02653700	C	0.09859600	-0.83953300	0.00000000
H	-1.83220200	-0.19212700	0.91722100	H	-1.20990200	0.64380900	-0.68056000	O	-0.44043000	-1.91539600	0.00000000
H	-1.83220200	-0.19212700	-0.91722100	H	-0.00677200	2.22535900	0.11689800	C	0.00000000	0.59913600	0.00000000
O	0.78207100	-1.73603100	0.00000000	O	1.89193300	-0.57029400	-0.01220400	N	-0.68277100	1.74259500	0.00000000
C	0.00000000	0.71273300	0.00000000	C	-0.63737900	-0.11613700	0.12663000	H	-1.68810800	1.73084400	0.00000000
N	0.38562000	1.90637100	0.00000000	N	-1.91228800	-0.43242300	0.02865100	H	2.28814800	0.16899000	0.00000000
H	1.40848200	1.94455800	0.00000000	H	-2.03661500	-1.42234600	-0.17736400	H	-0.21524000	2.63474600	0.00000000
3				3-TS				3-P			
C	-1.24711600	-0.13974400	0.00000000	C	-0.11152000	1.14996800	-0.01548500	C	1.21594700	0.08761600	0.00000000
C	0.13045100	-0.74243100	0.00000000	C	-0.64484700	-0.14854800	-0.13550200	C	0.00000000	0.62747700	0.00000000
H	-1.83220200	-0.19212700	0.91722100	H	-1.41650000	0.61194900	0.52030600	O	-0.75923900	1.70783500	0.00000000
H	-1.83220200	-0.19212700	-0.91722100	H	-0.17537800	2.22554600	-0.09482400	C	0.08051600	-0.79609400	0.00000000
O	0.78207100	-1.73603100	0.00000000	O	-1.80911200	-0.63144400	0.02024300	N	-0.34577400	-1.98556000	0.00000000
C	0.00000000	0.71273300	0.00000000	C	0.77844200	0.00928900	0.02066900	H	-1.36360900	-1.99743500	0.00000000
N	0.38562000	1.90637100	0.00000000	N	1.98271900	-0.35472500	0.03466900	H	-0.20696400	2.49957500	0.00000000
H	1.40848200	1.94455800	0.00000000	H	2.05328700	-1.36713000	-0.04820200	H	2.28612600	0.22010700	0.00000000
4				4-TS				4-P			
C	0.00000000	-0.74855300	0.00000000	C	0.81919100	-0.06730600	0.00473300	C	-0.82229300	-0.02707600	0.00009000
C	-0.21467400	0.71719900	0.00000000	C	-0.59752500	-0.27770600	0.03473100	C	0.58181300	-0.06132500	0.00011600
O	-0.77801800	1.75399700	0.00000000	O	-1.82777700	-0.43180600	-0.01437400	O	1.80675500	-0.50057800	-0.00001800
N	1.05375500	0.15453700	0.00000000	N	-0.14168000	0.98219600	0.00685300	N	0.00479600	1.10371100	-0.00002300
H	2.06408700	0.30335700	0.00000000	H	-1.44450700	0.98188800	-0.06791500	O	-1.93271400	-0.43081400	-0.00007300

O	-0.24102300	-1.90362100	0.00000000	O	1.96606100	-0.29159300	-0.01273100	H	2.41698100	0.25556100	-0.00033900
5				5-TS				5-P			
C	0.73091100	-0.05530300	-0.05345200	C	-0.81207500	0.01892800	0.00016100	C	0.81732200	-0.00103700	0.02166700
H	-0.00001100	1.97831300	0.46579300	H	2.61076400	0.21402700	0.00102900	H	-1.39130200	1.00166200	-0.33408900
N	0.00000000	1.12099900	-0.07932200	N	-0.02296200	1.16320000	-0.00001400	N	-0.13259400	0.99829700	0.03911000
C	-0.73091200	-0.05530000	-0.05346100	C	0.59447900	0.01510600	-0.00063600	C	-0.60172500	-0.27290800	0.17494200
N	-1.91281900	-0.44568700	0.05159600	N	1.84006100	-0.43809000	0.00029800	N	-1.86861000	-0.33672500	-0.07165000
H	-1.96272300	-1.46104500	0.00430900	H	2.03376500	-1.42406500	-0.00094600	H	-2.39141900	-1.20236700	-0.09147600
N	1.91282100	-0.44568400	0.05159300	N	-2.00229300	-0.38178000	0.00008100	N	2.03405200	-0.22570000	-0.08242800
H	1.96272900	-1.46104200	0.00431100	H	-2.04260000	-1.39748200	0.00020500	H	2.25920100	-1.20672800	0.05068700
1-W				1-W-TS				1-W-P			
C	0.21044500	-0.95884200	0.22482700	C	0.24245300	-0.82603500	0.57185100	C	0.56109800	-1.06071600	-0.00003200
C	1.46146200	-0.14094300	-0.02174200	C	1.32134200	-0.13065400	-0.07346600	C	1.65041900	-0.13726700	0.00000800
C	0.15121000	0.54278100	0.13993100	C	0.06807100	0.56284100	0.22483900	C	0.27652000	0.25727200	-0.00020600
O	2.63033000	-0.15998500	-0.21426500	O	2.47678200	-0.10987800	-0.38837300	O	2.82741500	0.10026600	0.00005100
H	-0.28653600	-1.55889800	-0.53744600	H	-1.05076800	-0.91070700	-0.10317600	H	-3.53740800	-0.41599400	-0.76996500
H	0.14182200	-1.38159800	1.23017600	H	0.09168200	-1.60331000	1.31782400	H	0.17356800	-2.06942100	0.00034400
O	-0.57973200	1.48040300	0.05739900	O	-0.80802400	1.41490000	0.12578400	O	-0.66220900	1.16928300	0.00002700
O	-2.65378600	-0.52315700	-0.14507800	O	-2.20329000	-0.64348000	-0.27264200	O	-2.97658400	-0.29284500	-0.00006100
H	-2.36678300	0.39258400	-0.04967600	H	-2.06523200	0.33998800	-0.08507900	H	-1.53703700	0.73118800	0.00009700
H	-3.60170400	-0.48815600	-0.28559600	H	-2.49062100	-0.75522000	-1.18706400	H	-3.53632500	-0.41513500	0.77077100
2-W				2-W-TS				2-W-P			
C	-0.20077600	-0.99039400	0.00137600	C	-0.21753600	-0.87267800	0.46329200	C	-0.78614100	-1.13884900	0.00028400
C	-1.46316500	-0.18549000	-0.00019700	C	-1.33957100	-0.16037900	-0.06217200	C	-1.77874500	-0.14746800	-0.00004200
H	0.10675100	-1.50075800	-0.91078700	H	1.05020400	-0.97332900	-0.20008400	H	3.84490800	-0.51992000	-0.76812800
H	0.10673200	-1.49958100	0.91417500	H	-0.11572300	-1.58180000	1.27992800	H	-0.47333400	-2.17224600	0.00040100
O	-2.65058900	-0.16889500	-0.00086800	O	-2.50396200	-0.11256500	-0.33417900	O	-2.92443500	0.23073000	-0.00038800
C	-0.17225200	0.51346600	-0.00018500	C	-0.09638000	0.55579200	0.23754000	C	-0.36986000	0.15651000	0.00023400
N	0.63005900	1.48061800	0.00075400	N	0.86361400	1.40440300	0.19069100	N	0.66218100	0.99268500	0.00032700
H	0.13648500	2.37553500	-0.00040700	H	0.60801900	2.26579300	-0.28447000	H	0.49420400	1.98391300	-0.00000800
O	2.68767000	-0.54167200	-0.00071700	O	2.19533400	-0.63454200	-0.41972800	O	3.37997000	-0.17997100	-0.00024100
H	2.31997300	0.35348600	0.00093900	H	2.00211400	0.35452700	-0.13125800	H	1.61757300	0.65230600	0.00044900
H	3.64016400	-0.43395800	-0.00248200	H	2.80002800	-1.05556400	0.20034300	H	3.84558100	-0.52008100	0.76716900
3-W				3-W-TS				3-W-P			
C	0.18102500	-1.00141600	-0.00146900	C	0.19772000	-0.88342100	0.51525900	C	0.54626100	-1.09612700	0.00018800
C	0.13236300	0.49071800	-0.00134900	C	0.05281600	0.50207800	0.26523800	C	0.25107900	0.20480500	-0.00007300
H	-2.33829700	0.41863900	0.00052200	H	-2.00161900	0.40391600	-0.07201400	H	-1.54506300	0.73969900	0.00008800
H	-0.11658500	-1.51723400	0.91068500	H	0.05375500	-1.67670400	1.24093000	H	0.20176700	-2.11784100	-0.00007200
O	-0.56118900	1.46305500	-0.00040400	O	-0.79926800	1.38824900	0.16042100	O	-0.65809600	1.15061200	0.00016300
C	1.43755200	-0.16753800	-0.00002200	C	1.30883900	-0.14757900	-0.05118600	C	1.63138300	-0.15882600	-0.00008400
N	2.69033800	-0.23110700	0.00172800	N	2.53710900	-0.18027700	-0.34719000	N	2.88483900	0.02855100	-0.00005600
H	3.08983400	0.71127800	0.00155500	H	2.84332800	0.73983600	-0.66161200	H	3.08908500	1.02585500	-0.00018200
O	-2.71323700	-0.47037100	0.00109600	O	-2.24272200	-0.57295600	-0.29531300	O	-3.01356800	-0.24744700	-0.00008600
H	-0.11294100	-1.51579700	-0.91568100	H	-1.11876600	-0.92605600	-0.16824200	H	-3.56938100	-0.38564300	-0.77082500
H	-3.66460700	-0.35119500	0.00232800	H	-2.55679100	-0.62787100	-1.20545000	H	-3.56930400	-0.38635200	0.77057900
4-W				4-W-TS				4-W-P			
C	-1.42137600	-0.12116100	0.00003100	C	1.37066800	-0.08429000	-0.00295600	C	-1.46802000	-0.13346400	0.00132600
C	-0.14203100	0.62293600	-0.00015200	C	0.10332600	0.59889400	-0.00589100	C	-0.20348500	0.48390500	0.00050200
O	0.62493400	1.53286800	-0.00002100	O	-0.81602000	1.41335800	-0.00654000	O	0.72063100	1.38226600	0.00290000
N	-0.18031600	-0.74431900	-0.00018000	N	0.15074900	-0.75129500	0.00341800	N	-0.25557500	-0.82475100	-0.00317000
H	0.43823400	-1.56024500	-0.00079300	H	-1.14244200	-1.10805100	0.03372600	H	1.93347500	-1.29340500	0.00324900
O	-2.58127200	-0.33613000	0.00016700	O	2.54259300	-0.24626900	-0.00668900	O	-2.64833100	-0.22980000	0.00409800
O	2.50562100	-0.66427000	0.00021000	O	-2.22460800	-0.68120500	0.08817000	O	2.53795000	-0.54024000	-0.03381500
H	2.35402400	0.29017700	0.00017700	H	-1.97661000	0.32066400	0.04446800	H	1.59049000	0.90807000	0.00123100
H	3.45613000	-0.79009500	-0.00023700	H	-2.79587200	-0.92824700	-0.64855800	H	3.41209100	-0.84185600	0.22128500
5-W				5-W-TS				5-W-P			
C	-1.37525500	-0.15589600	0.03043400	C	-1.34776700	-0.12768000	0.01081000	C	-1.43007900	-0.19930900	0.00046800
H	2.29301300	0.22987000	-0.13698600	H	2.01484800	0.29954900	-0.08843200	H	1.68290300	1.18434800	0.00182900
N	-0.18216800	-0.72948600	0.41850400	N	-0.13163000	-0.75848500	0.10750500	N	-0.19975500	-0.83635600	0.00075300
C	-0.13548700	0.61234100	0.15409900	C	-0.09702600	0.59000200	0.05839400	C	-0.19054500	0.47432000	0.00124400

N	0.72140800	1.52404600	0.03410700	N	0.89947900	1.39936600	0.01529700	N	0.69943800	1.44597000	0.00282600
H	0.29414200	2.41607400	-0.19802100	H	0.66425700	2.37993700	-0.06420300	H	0.41273300	2.40891200	-0.00143000
N	-2.55287700	-0.46076200	-0.25337900	N	-2.57837400	-0.35257100	-0.05734900	N	-2.66900400	-0.40649700	-0.00002300
H	-3.09519400	0.37044100	-0.47721400	H	-3.09892400	0.51921200	-0.10287000	H	-3.18092400	0.47159000	0.00035500
O	2.47653400	-0.72137700	-0.19096600	O	2.23157400	-0.73400300	-0.14595000	O	2.59424700	-0.60022400	-0.01614500
H	0.43899300	-1.50481300	0.18747700	H	1.10435500	-1.12291000	-0.03211800	H	1.84815800	-1.21676300	-0.00624400
H	3.41668500	-0.81581200	-0.34935700	H	2.80529400	-0.99586500	0.58181900	H	3.39214200	-1.11817300	0.09949000

POLYRATE INPUT file

File.70	File.71
*GRGENERAL	#m062x/6-311+G(d,p) FCHK OPT
GRRESTART on	8-reactant
*GRCOMMON	0 1
GRENER	C0.73091100-0.05530300-0.05345200
%mem=12gb	H-0.000011001.978313000.46579300
%nproc=12	N0.000000001.12099900-0.07932200
#m062x/6-311+G(d,p) FCHK UNITS=AU NOSYMM	C-0.73091200-0.05530000-0.05346100
END	N-1.91281900-0.445687000.05159600
GRFIRST	H-1.96272300-1.461045000.00430900
%mem=12gb	N1.91282100-0.445684000.05159300
%nproc=12	H1.96272900-1.461042000.00431100
#m062x/6-311+G(d,p) FORCE FCHK UNITS=AU NOSYMM	
END	
GRSEC	
%mem=12gb	
%nproc=12	
#m062x/6-311+G(d,p) FREQ=NORAMAN FCHK UNITS=AU	
NOSYMM	
END	
*GRPATH	
GRENER	
%mem=12gb	
%nproc=12	
#m062x/6-311+G(d,p) FCHK UNITS=AU NOSYMM	
END	
GRFIRST	
%mem=12gb	
%nproc=12	
#m062x/6-311+G(d,p) FORCE FCHK UNITS=AU NOSYMM	
END	
GRSEC	
%mem=12gb	
%nproc=12	
#m062x/6-311+G(d,p) FREQ=NORAMAN FCHK UNITS=AU	
NOSYMM	
END	
File.73	File.75
#m062x/6-311+G(d,p) FCHK OPT	#m062x/6-311+G(d,p) OPT=(TS,NOEIGENTEST,CALCFC) FCHK
8-pdt	Saddle Point 8-W
0 1	0 1
C-0.812075000.018928000.00016100	C0.81732200-0.001037000.02166700
H2.610764000.214027000.00102900	H-1.391302001.00166200-0.33408900
N-0.022962001.16320000-0.00001400	N-0.132594000.998297000.03911000
C0.594479000.01510600-0.00063600	C-0.60172500-0.272908000.17494200
N1.84006100-0.438090000.00029800	N-1.86861000-0.33672500-0.07165000
H2.03376500-1.42406500-0.00094600	H-2.39141900-1.20236700-0.09147600
N-2.00229300-0.381780000.00008100	N2.03405200-0.22570000-0.08242800
H-2.04260000-1.397482000.00020500	H2.25920100-1.206728000.05068700

File.dat	
*GENERAL TITLE Proton tunneling in 8 END ATOMS 1 C 2 H 3 N 4 C 5 N 6 H 7 N 8 H END NOSUPERMOL *SECOND HESSCAL hhook FPRINT *OPTIMIZATION PRINT OPTMIN ohook OPTTS ohook *REACT1 STATUS 0 INITGEO hooks GEOM 1 2 3 4 5 6 7 8 END SPECIES nonlinrp *PROD1 STATUS 0 INITGEO hooks GEOM 1 2 3 4 5 6 7 8 END SPECIES nonlints *START STATUS 0	

INITGEO hooks

GEOM

1

2

3

4

5

6

7

8

END

SPECIES nonlints

PROJECT

*PATH

SCALEMASS 1.00

RODS ON

INTMU 3

NSTEPS 99999

SSTEP 0.002

INH 10

RPM pagem

SRANGE

SLP 2.5

SLM -2.5

END

SIGN reactant

#COORD curv3

IDIRECT 1

PRPATH

coord 3 2 5 2

xmol

freq 3 4 6

END

INTDEF

1-3

1-4

1-7

2-3

3-4

4-5

5-6

7-8

1-3-2

1-3-4

1-4-5

1-7-8

3-1-7

1-3-4-5

1-4-5-6

2-3-4-5

3-1-4-5

3-1-7-8

END

*TUNNEL

ZCT

SCT

*RATE

FORWARDK

SIGMAF 1 TST CVT PRDELG PRPART rtp TEMP 50 75 100 125 150 175 200 225 250 273 275 298 300 325 350 375 400 425 450 500 1000 1500 2000 END ANALYSIS 50 75 100 125 150 175 200 225 250 273 275 298 300 325 350 375 400 425 450 500 1000 1500 2000 END EACT 75. 100. 125. 150. 175. 200. 225. 250. 273. 298. 325. 350. 375. 400. END GTLOG	

